Sulfaguanidine 57-67-0 | DTXSID1023609

Model Performance

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Model	I)ata
Widdei	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 189 °C

Global applicability domain: Outside

Local applicability domain index: 2.83e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

Image not found
Sulfaguanidine
Measured: 192
Predicted: 189

Image not found Carbarsone Measured: 174 Predicted: N/A Image not found Guanfacine Measured: 226 Predicted: 218

Image not found
Carbutamide

Measured: 145
Predicted: 153

Image not found

Flupirtine
Measured: 116
Predicted: 216